**Rules in InChI Source Code**

**Rule # 1: (ichi\_bns.c -> Line Nr. 5454)**

Ring system with radicals is transferred to aromatic ring system. As shown in the comparison figures below, figure 1.1 is a simple ring system with radical and figure 1.2 is the converted aromatic system as interpreted by InChI.

A hexagon with lines and dots

Description automatically generated A hexagon with lines and letters

Description automatically generated

Figure 1.1 Figure 1.2

The above mentioned rule is verified by generation of this unique InChI key as given in bold.

“**InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H**”.

**Rule # 2: (ichi\_bns.c -> Line Nr. 5516)**

Removing protons from NH(+) but not PH(+) and adding protons to COO(-) or removing protons from COOH to make the organic part neutral.

Example for a de-protonation process is a compound named as “Cyclohexylammonium Chloride” which is composed of cyclohexylammonium cation (C6H11NH3+) and a chloride anion (Cl-). After the de-protonation process is completed we have cyclohexylamine and a proton. Hence, the charge from N (+1) changes to N (0). Figure 2.1 shows the results of the de-protonation during normalization. The output is generated into a command line terminal.

Another example is of Zwitter ion which are commonly found in amino acids and other molecules which have both acidic and basic functional groups. When a zwitter ion undergoes protonation it gains a proton on to a carboxyl group (-COOH) to become neutral. Figure 2.2 shows the results of the protonation process.

A screenshot of a computer

Description automatically generated

Figure 2.1 : Shows the process of de-protonation with Nitrogen atom.

A screenshot of a computer program

Description automatically generated

Figure 2.2 : Shows the process of protonation with the Carboxyl group.